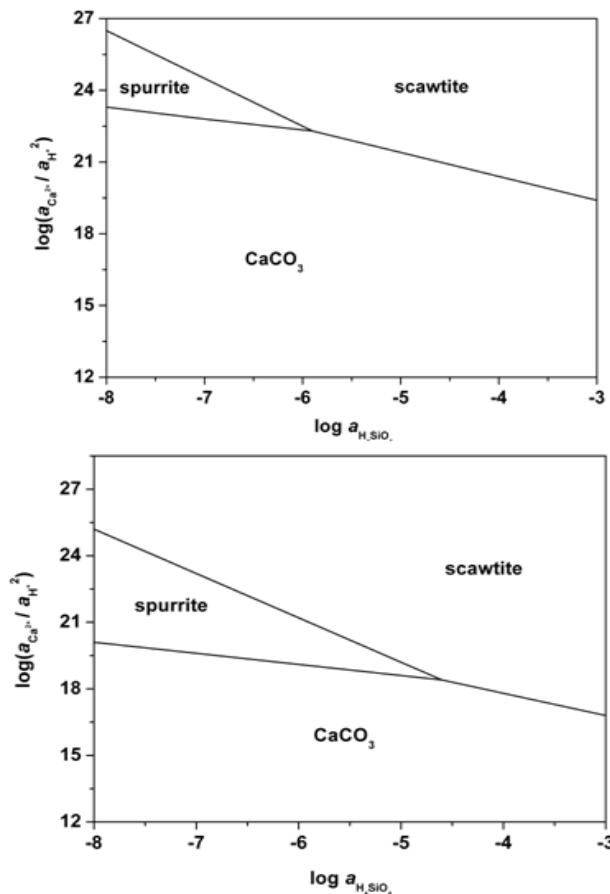




Thermochemistry of two calcium silicate carbonate minerals: scawtite, $\text{Ca}_7(\text{Si}_6\text{O}_{18})(\text{CO}_3) \cdot 2\text{H}_2\text{O}$, and spurrite, $\text{Ca}_5(\text{SiO}_4)_2(\text{CO}_3)$



Mineral stability diagram at 25 and 80 °C for $\text{CaO-SiO}_2\text{-H}_2\text{O-CO}_2$ system

Scientific Achievement

Spurrite-scawtite- CaCO_3 stability diagrams suggest that spurrite forms in strongly oversaturated calcium solutions with a low aqueous silica activity at 25 °C. Scawtite could precipitate in a range of $\text{Ca}^{2+}/\text{H}^+$ ratio, high H_2SiO_4 activity and in saturated quartz.

Significance and Impact

scawtite and spurrite may precipitate near caprocks with dissolving silicate minerals, clays, or cement phases. At 80 °C relevant to CO_2 sequestration, the expanded scawtite and spurrite stability fields suggest their favorable formation over calcite under moderate calcium concentration and pH by direct carbonation reactions

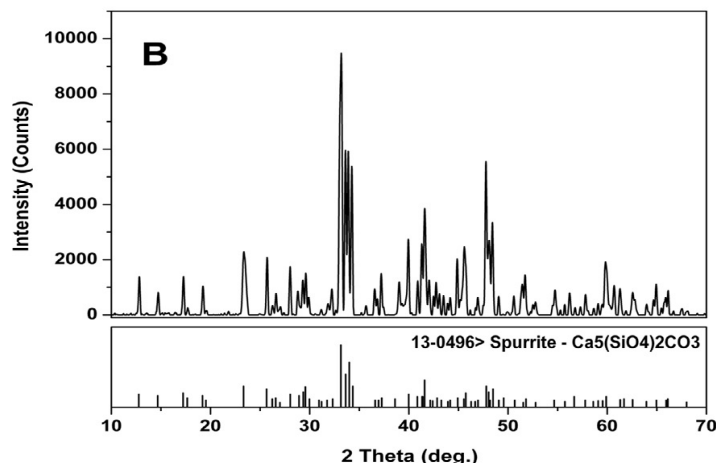
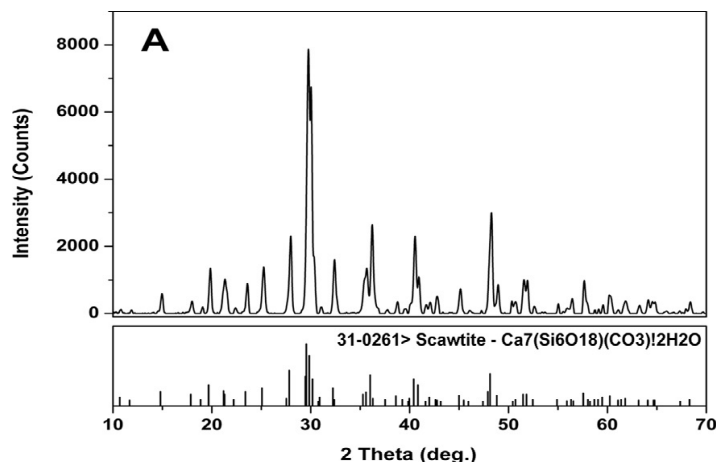
Research Details

Calcium silicate carbonate minerals, scawtite, $\text{Ca}_7(\text{Si}_6\text{O}_{18})(\text{CO}_3) \cdot 2\text{H}_2\text{O}$, and spurrite, $\text{Ca}_5(\text{SiO}_4)_2(\text{CO}_3)$, were synthesized and characterized. Their enthalpies of formation were determined by high temperature oxide melt solution calorimetry

Yin-Qing Zhang, A.V. Radha, Alexandra Navrotsky
Geochimica et Cosmochimica Acta 115 (2013) 92–99



Thermochemistry of two calcium silicate carbonate minerals: scawtite, $\text{Ca}_7(\text{Si}_6\text{O}_{18})(\text{CO}_3) \cdot 2\text{H}_2\text{O}$, and spurrite, $\text{Ca}_5(\text{SiO}_4)_2(\text{CO}_3)$



Powder XRD patterns of (A) Scawtite and (B) spurrite

Structures

Spurrite is an orthosilicate having separate layers of silicate and carbonate groups due to their different Lewis-base strengths. scawtite composed of a $[\text{CaO}_6\text{-}8]$ polyhedral sheet linked by Si_6O_{18} rings and isolated CO_3 groups parallel to (101)

Enthalpies of formation

The enthalpy of formation from the oxides is -689.5 ± 14.3 kJ/mol for scawtite and -455.1 ± 9.7 kJ/mol for spurrite, and the enthalpy of formation from the elements is -11564.5 ± 16.8 kJ/mol for scawtite and -5845.5 ± 10.9 kJ/mol for spurrite.



Thermochemistry of two calcium silicate carbonate minerals: scawtite, $\text{Ca}_7(\text{Si}_6\text{O}_{18})(\text{CO}_3) \cdot 2\text{H}_2\text{O}$, and spurrite, $\text{Ca}_5(\text{SiO}_4)_2(\text{CO}_3)$

Thermodynamic equilibrium constants of the chemical reactions used to construct log–log diagram of $\text{Ca}^{2+}/\text{H}^+$ activity vs. H_4SiO_4 activity in the $\text{CaO}\text{--}\text{SiO}_2\text{--}\text{H}_2\text{O}\text{--}\text{CO}_2$ system.

Reaction	log relation	log K at T	
		25 °C	80 °C
$\text{Ca}_7(\text{Si}_6\text{O}_{18})\text{CO}_3 \cdot 2\text{H}_2\text{O} (\text{s}) + 4\text{H}_2\text{O} (\text{l}) + 12\text{H}^+ (\text{aq}) = 6\text{Ca}^{2+} (\text{aq}) + 6\text{H}_4\text{SiO}_4 (\text{aq}) + \text{CaCO}_3 (\text{s})$	$6 \log (a_{\text{Ca}^{2+}} / a_{\text{H}^+}^2) = \log K - 6 \log a_{\text{H}_4\text{SiO}_4}$	98.1	82.6
$\text{Ca}_5(\text{SiO}_4)_2\text{CO}_3 (\text{s}) + 8\text{H}^+ (\text{aq}) = 4\text{Ca}^{2+} (\text{aq}) + 2\text{H}_4\text{SiO}_4 (\text{aq}) + \text{CaCO}_3 (\text{s})$	$4 \log (a_{\text{Ca}^{2+}} / a_{\text{H}^+}^2) = \log K - 2 \log a_{\text{H}_4\text{SiO}_4}$	77.1	64.2
$\text{Ca}_7(\text{Si}_6\text{O}_{18})\text{CO}_3 \cdot 2\text{H}_2\text{O} (\text{s}) + 4\text{H}_2\text{O} (\text{l}) + 4\text{H}^+ (\text{aq}) = \text{Ca}_5(\text{SiO}_4)_2\text{CO}_3 (\text{s}) + 4\text{H}_4\text{SiO}_4 (\text{aq}) + 2\text{Ca}^{2+} (\text{aq})$	$2 \log (a_{\text{Ca}^{2+}} / a_{\text{H}^+}^2) = \log K - 4 \log a_{\text{H}_4\text{SiO}_4}$	21.0	18.4